Boltzmann entropy and chaos in a large assembly of weakly interacting systems

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Abstract

We introduce a high dimensional symplectic map, modeling a large system consisting of weakly interacting chaotic subsystems, as a toy model to analyze the interplay between single-particle chaotic dynamics and particles interactions in thermodynamic systems. We study the growth with time of the Boltzmann entropy, S_B, in this system as a function of the coarse graining resolution. We show that a characteristic scale emerges, and that the behavior of S_B vs t, at variance with the Gibbs entropy, does not depend on the coarse graining resolution, as far as it is finer than this scale. The interaction among particles is crucial to achieve this result, while the rate of entropy growth depends essentially on the single-particle chaotic dynamics (for t not too small). It is possible to interpret the basic features of the dynamics in terms of a suitable Markov approximation.

Keywords: Boltzmann entropy, irreversibility, chaotic dynamics, ensembles.

1 Introduction

Statistical mechanics was founded by Maxwell, Boltzmann and Gibbs for systems with a very large number of particles. Given their different approaches, Boltzmann and Gibbs are often considered as the champions of two different points of view about statistical mechanics. This common *vulgata* takes Gibbs as the founder of the ensemble approach, and Boltzmann as the promoter of a dynamical theory based on the ergodic hypothesis; according to this tradition, modern textbooks [1] use Gibbs's terminology for the ensembles (i.e. microcanonical, canonical and grand-canonical). Actually, both ergodicity and ensembles are Boltzmann's inventions; more detailed discussions about Boltzmann, Gibbs, and the origin of the statistical mechanics are contained in the absolutely recommendable book by Cercignani [2], and the papers by Klein [3], Lebowitz [4], and Gallavotti [5].

The Gibbs' approach to statistical mechanics uses the general concept of ensembles without any reference to the precise origin of such an idea. The relevant literature is huge [6, 3] : sometimes the ensembles are derived from philosophical considerations, other times from information-theoretic, and even from anthropocentric considerations. In Van Kampen's words, sometimes this produces *a slightly mystic aura*, which diverts the attention away from the physical meaning of the ensemble theory [7].

Ergodic theory begins with Boltzmann's attempt to justify the determination of average values in kinetic theory [8, 5]. Macroscopic systems contain a very large number (of the order of the Avogadro's number) of particles; this implies the practical necessity of a statistical description. Since in any macroscopic observation the time scale is much larger than the microscopic time scale, over which the molecular changes take place, an experimental measurement is actually the result of an observation on a single system, during which it goes through a very large

number of microscopic states. Thus, one may assume that the outcome of the measurement of an observable $A(\mathbf{X})$ is an average performed over all these states:

$$\overline{A}^T(\mathbf{X}_0) = \frac{1}{T}\int_{t_0}^{t_0+T} A(\mathbf{X}(t;\mathbf{X}_0))\mathrm{d}t\,, \tag{1}$$

where the vector

$$\mathbf{X}(t;\mathbf{X}_0) \equiv (\mathbf{q}_1(t;\mathbf{X}_0),\ldots,\mathbf{q}_N(t;\mathbf{X}_0),\mathbf{p}_1(t;\mathbf{X}_0),\ldots,\mathbf{p}_N(t;\mathbf{X}_0)) \tag{2}$$

lies in the $6\,N$ - dimensional phase space Γ, gives the state of the system at time t and, in general, depends on the initial state $\mathbf{X}_0$. According to the usual notation, the components of $\mathbf{X}$, $\mathbf{q}_i$ and $\mathbf{p}_i$, indicate the position and momentum vectors of the i-th particle.

Obviously, it is impossible to obtain the complete description $\mathbf{X}_0$ of the microscopic state of the system at the initial time, for such high-dimensional systems as those relevant in statistical mechanics. This means that, if $\overline{A}^T$ depends too strongly on the initial condition, no statistical predictions can be made, independently of how difficult it may be to integrate the equations of motion. The ergodic hypothesis allows us to overcome this obstacle, stating that for sufficiently large T, the average $\overline{A}^T$ depends only on the system energy, in the sense that it takes the same values for *almost all*[1] the trajectories on the given constant energy surface. This allows us to identify the time average with a phase space average:

$$\overline{A} \equiv \lim_{T\to\infty}\frac{1}{T}\int_{t_0}^{t_0+T} A(\mathbf{X}(t;\mathbf{X}_0))\mathrm{d}t = \int A(\mathbf{X})P_{mc}(\mathbf{X})\mathrm{d}\mathbf{X} \equiv \langle A\rangle \tag{3}$$

where P_{mc} is the microcanonical probability density, except for a negligible set of initial conditions. The validity of such an equality eliminates the necessity of determining the initial state of the system, and of solving the Hamilton's equations. Whether (3) is valid or not, i.e. whether it is possible to substitute the temporal average with an average in phase space, constitutes the essence of the ergodic problem in physics. The relevance of this issue is evident: let the statistical properties of a large isolated system be properly described by the microcanonical ensemble, then it is not difficult to show that a small part of the given system, which is still large at the microscopic scale, is described by the canonical ensemble.

We stress that, in this context, the ensemble is just a useful mathematical tool, and one should not forget that thermodynamics, as a physical theory, is developed to describe the properties of *single* systems, made of many microscopic, interacting parts. Although some may find hard to distinguish between "thermodynamic systems" and other systems of interest in statistical physics, in this paper, when referring to a thermodynamic system, we have in mind a system that is characterized by macroscopic properties such as its temperature, while many other, equally

[1]Here, *almost all* has a technical meaning, i.e. it refers to all trajectories, except those which originate in a set of vanishing phase space volume.

interesting physical systems, do not even need to have a temperature. The distinction makes sense because different laws describe the behaviour of the different systems.

To justify eq. (3) in physical systems, Khinchin's point of view clearly states that the success of statistical mechanics techniques is mainly due to the many degrees of freedom, while the underlying dynamics play only a minor role. In his celebrated book *Mathematical Foundations of Statistical Mechanics* [9], he presents some important results on the ergodic problem which do not rest on the metrical transitivity of the dynamics, which (3) requires. Khinchin's idea on the ergodic problem in statistical mechanics is that one should profit from the fact that macroscopic systems have a large number of degrees of freedom, and that the physical observables for which (3) is required to hold are not generic regular functions, as in the dynamical systems approach to ergodicity. In other words, taking into account the large number of degrees of freedom should be enough to obtain the validity of the equivalence between time averages and ensemble averages for the small class of relevant observables. Moreover, it is fair for physical purposes to accept the failure of the ergodic hypothesis for a set of initial conditions $\mathbf{X}_0$ which is a negligible fraction of the phase space, or that becomes negligible when $N \to \infty$. In a nutshell, Khinchin's point of view is that statistical mechanics works independently of the mathematical validity of the dynamical systems notion of ergodicity, because the physically relevant observables are practically constant, except in an irrelevant region of the constant energy surface. This makes marginal the role of the dynamics, for equilibrium states, and the existence of good statistical properties is mainly due to the large number of degrees of freedom, i.e. to $N \gg 1$.

The ergodic approach, whether in its strong or its weak version, is a natural way to introduce probabilistic concepts in a deterministic context: in experimental situations one deals with a unique system with many degrees of freedom, whose microstates explore with given frequency the different regions of the phase space. Consequently, the ergodic hypothesis seems to provide the appropriate tools for the equilibrium statistical mechanics to be founded on physical grounds, using a frequentistic interpretation of the probability distributions.

The other way of connecting probability and dynamics (which does not contrast with Boltzmann's point of view) is to take into account the unavoidable uncertainty on the initial conditions. This approach, originally due to Maxwell, considers that there are *a great many systems the properties of which are the same, and that each of these is set in motion with a different set values for the coordinates and momenta* [10].

The discovery of deterministic chaos, implying that even deterministic systems with a few degrees of freedom may present some statistical features typical of probabilistic evolutions, forced the physicists to reconsider from a new perspective the foundations of statistical mechanics [11]. Moreover one may also find useful to define, formally, "thermodynamic" system any system with ergodic dynamics such that (3) applies. In this paper we will consider only systems with many degrees of freedom, such that, usually, the thermodynamic observables have negligible fluc-

tuations.

The situation is much more intricate for the non equilibrium problems than for equilibrium ones, and even after many years of debate, there is no general agreement about the fundamental ingredients needed for statistical mechanics to hold.

The aim of this paper is to give a contribution for the understanding of the role of deterministic chaos, and of coarse-graining procedures, in non equilibrium statistical mechanics. In particular the paper concerns the problem of the growth of entropy. These issues are the source of heated debates, on which only partial agreement has been reached within the statistical mechanics community. Recent examples of this are given by the debate on irreversibility originated by Lebowitz's paper [4], and the partly contrasting views on irreversible entropy production reported in [12, 13, 14, 15].[2]

Our results support the view that systems of many noninteracting chaotic particles may properly describe, for some aspects, highly rarefied gases, or Knudsen gases in an irregular container, even if a normal thermodynamic behavior may be absent.[3] This is a very delicate issue: it is known [18, 19] that some form of irreversibility may be found in systems of non interacting particles. For example, free particles in a box show homogenization of the spatial coordinates; in irregularly shaped boxes the distribution of velocity can become isotropic; but, in the absence of interactions, a relaxation of velocities to a Maxwellian (that we call, as noted above, a *normal thermodynamic behaviour*) is impossible. We find, in fact, that the Γ or μ space graining required for noninteracting particle systems to look thermodynamic-like have an equally arbitrary character, with no physical meaning, and play an essentially identical role in both spaces.

Differently, we are going to show in this paper that, in the case of interacting chaotic particles, a characteristic scale naturally emerges in the μ space. This may be interpreted as the scale at which the diffusive, small scale behavior due to the interaction first smoothes the fragmented structures created by the chaotic dynamics. In this case, the coarse graining in μ-space shows completely different features from the coarse graining in Γ space: in particular, the growth of the Boltzmann entropy results independent of the resolution, as long as the observation scale is finer than the characteristic scale. We stress that to achieve this result, it is of fundamental importance that the number of particles must be large, which is not required for the coarse graining in Γ-space.

These facts are reflected in the different nonequilibrium behaviours of the Boltzmann and Gibbs entropies. Indeed, the constancy of the Gibbs entropy can be

[2] As a matter of fact, the views expressed in Refs.[13] are not particularly contrasting with those of Refs.[14], as they all require the condition of local thermodynamic equilibrium, and do the coarse graining in μ-space rather than in Γ-space.

[3] The lack of interactions imparts very interesting and useful (cf. Ref.[16, 17]) properties to such gases, not their number density. Therefore, the behaviour of a system of noninteracting particles, like that of a Knudsen gas, is dominated by the collisions with the walls of its container, even if its number of particles per unit volume is high.

consistently accommodated in this framework. If one accepts, as we do, that the Gibbs canonical ensemble does yield the correct equilibrium thermodynamics, then the dynamical invariance of the Gibbs entropy may provide a simple interpretation of the second law of thermodynamics [20]. One considers the ensemble of points in Γ space, that are compatible with the values of the macroscopic variables $\{A_k\}$, defining the initial equilibrium thermodynamic state, and that are weighted by the suitable Gibbs density $\rho(\mathbf{X})$. For large systems, the quantity $H_G(\{\rho\}) = \int \rho(\mathbf{X}) \ln \rho(\mathbf{X}) \mathrm{d}\mathbf{X}$ allows to determine a phase space region R, whose volume is $\Delta\Gamma = \exp[-H_G(\{\rho\}]$, containing the "reasonably probable" microstates. As a consequence of an adiabatic change of state, the microstates in R evolve, and after a sufficiently long time T, so that a new equilibrium is attained, they occupy the new region R_T, whose volume, because of the Liouville equation, is still $\Delta\Gamma$. However, the quantities defining the new thermodynamic equilibrium are $\{\widetilde{A}_k\}$, evolved from $\{A_k\}$. These values define the new Gibbs density $\widetilde{\rho}(\mathbf{X})$, with a support essentially contained in a region $\widetilde{R}$ of volume $\Delta\widetilde{\Gamma} = \exp[-H_G(\{\widetilde{\rho}\}]$. Since we accept that, at equilibrium, $S = -k_{_B} \int \rho(\mathbf{X}) \ln \rho(\mathbf{X}) \mathrm{d}\mathbf{X} = -k_{_B} H_G(\{\rho\}) = k_{_B} \ln \Delta\Gamma$, the second law of thermodynamics requires that $\Delta\widetilde{\Gamma} \geq \Delta\Gamma$. What is important to note here is that $\widetilde{\rho}(\mathbf{X})$, and therefore $\Delta\widetilde{\Gamma}$, is not determined by the evolution of the initial $\rho(\mathbf{X})$, it is constructed by the evolved values of the macrovariables $\{A_k\}$. A demonstration of the second law in statistical mechanics, in this framework, is equivalent to show that the microstates, compatible with the set of macroscopic variables, suitable to describe the thermodynamic system at hand, during an adiabatic evolution occupy phase-space regions of increasing volumes [21]. This fact guarantees the experimental reproducibility of the process. On the other hand, as Jaynes writes [20], "Any really satisfactory demonstration of the second law must therefore be based on a different approach than coarse-graining [of ρ]", since "the decrease of $\overline{H}$ [a coarse-grained version of $H_G(\{\rho\})$] is due only to the artificial coarse-graining operation and it cannot therefore have any physical significance...".

In the case of a dilute gas, a useful macroscopic variable to define the thermodynamic state of the system, is the single particle distribution function $f(\mathbf{q}, \mathbf{p}, t)$. In this case, and only in this case, the logarithm of the volume occupied by the compatible microstates is given by minus the Boltzmann H-function: $H_B = \int f(\mathbf{q}, \mathbf{p}, t) \ln f(\mathbf{q}, \mathbf{p}, t) \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}$. So, for a dilute gas, while the Gibbs entropy, as always, is expected to be constant, the Boltzmann entropy takes the form: $S_B = -k_{_B} \int f(\mathbf{q}, \mathbf{p}, t) \ln f(\mathbf{q}, \mathbf{p}, t) \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}$ and is expected to increase, as Lanford [22] demonstrated to be true, in a suitable limit.

Most of the ideas discussed in the present paper are known. See, for instance, [21] for the graining in phase space induced by a graining in μ-space and the choice of macro-variables, and for the relation between the one-particle distribution function of interacting and of noninteracting particle systems. Here, we express in a quantitative form, for a specific model, the qualitative statements made elsewhere, and we observe the existence of an intrinsic scale for the graining in the μ-space of interacting particle systems.

This paper is organized as follows. Section II is devoted to a brief summary of some basic facts about Gibbs and Boltzmann entropy and the link between deterministic chaos and statistical mechanics. In section III we introduce a symplectic map simulating the time evolution of a large system, consisting of weakly interacting chaotic subsystems, and we show the behavior of the Boltzmann entropy S_B vs time. The main result is that, for interacting systems, S_B is independent of the details of the coarse-graining procedure in μ-space, if the graining is sufficiently fine, i.e. the existence of an intrinsic graining scale in μ-space. The most remarkable fact is that some numerical aspects (e.g. the slope of S_B for large enough t) basically depend only on the chaotic properties of the single subsystem, but the presence of the coupling is absolutely necessary. In section IV we show how one can interpret the results with a mechanism similar to that used for the decoherence in the semiclassical limit of quantum mechanics. Conclusions and perspectives are in section V.

2 On the Gibbs and Boltzmann entropy

Let us consider a Hamiltonian system of N particles, and the vector $\mathbf{X}(t)$ which defines the microscopic state of the system. Denoting by $\rho(\mathbf{X})d\mathbf{X}$ the probability for the microscopic state to be found in the phase space volume $d\mathbf{X}$, one defines the Gibbs entropy:

$$S_G(\{\rho\}) = -k_{_B} \int \rho(\mathbf{X}) \ln \rho(\mathbf{X}) \mathrm{d}\mathbf{X} \tag{4}$$

where $k_{_B}$ is the Boltzmann's constant. Since the time evolution $\mathbf{X}(0) \to \mathbf{X}(t)$ is ruled by the Hamilton equations, the Liouville theorem implies that S_G does not change in time. However, a coarse graining of ρ by cells of size Δ in the Γ space (the microscopic phase space) leads to an increase of the coarse-grained Gibbs entropy[4]

$$S_G(t, \Delta) = -k_{_B} \sum_i p_\Delta(i,t) \ln p_\Delta(i,t) \ , \tag{5}$$

where the coarse-grained probability $p_\Delta(i,t)$ is given by:

$$p_\Delta(i,t) = \int_{\Lambda_{i,\Delta}} \rho(\mathbf{X},t) \mathrm{d}\mathbf{X} \ , \tag{6}$$

and $\Lambda_{i,\Delta}$ is the cell in the space Γ of linear size Δ centered in the point $\mathbf{X}^{(i)}$. When the system is chaotic, and the initial probability distribution is supported over a small region of linear size σ, simple arguments suggest that $S_G(t,\Delta)$ increases

[4]It is worth recalling that $S_G(t,\Delta)$ is the discretization of S_G, by cells of size Δ, except for an additive term $k_{_B} \ln \Delta$. At fixed Δ, the term is constant and not relevant if one considers the entropy differences with respect to the initial values.

linearly in time, after a short transient of length t_λ

$$S_G(t,\Delta) - S_G(0,\Delta) \simeq \begin{cases} 0 & t < t_\lambda \\ h_{KS}(t - t_\lambda) & t \geq t_\lambda \end{cases} \tag{7}$$

where h_{KS} is the Kolmogorov-Sinai entropy of the system,

$$t_\lambda \sim \frac{1}{\lambda_1} \ln\left(\frac{\sigma}{\Delta}\right) \tag{8}$$

and λ_1 is the first Lyapunov exponent of the Hamilton equations. The prediction of Eq (7) is not always completely correct; actually, it is valid only when intermittency effects are negligible [23]. To make things simpler we will assume the validity of Eq.(7), as commonly done in the presence of chaotic dynamics. Many consider Eq. (7) as a proof of the deep connection between chaos and irreversibility. Nevertheless, the result of Eq.(7) does not have a genuine thermodynamic character. This can be understood as follows:

a) the quantity $S_G(t,\Delta)$ describes properties of the Γ space that can not be computed from a single-system measurement;

b) the time increase of $S_G(t,\Delta)$ depends on the coarse-graining procedure and this appears as a non-ontological result;

c) the result of Eq.(7) is valid also for a generic, low-dimensional system - notice that one obtains the same result even in the case of chaotic non-interacting particles.

Consider now the Boltzmann point of view, for a system of N weakly interacting particles. The one-body probability distribution function $f(\mathbf{q},\mathbf{p},t)$, i.e. the probability density of finding a particle in a given volume of the μ space (the single-particle space) can be introduced without any reference to an ensemble of macroscopically identical systems, each represented by a point in Γ space. In fact, take a single system made of a large number N of identical particles, consider the discrete distribution

$$f(\mathbf{q},\mathbf{p},t) = \frac{1}{N}\sum_{i=0}^{N} \delta\left(\mathbf{q} - \mathbf{q}_i(t)\right)\delta(\mathbf{p} - \mathbf{p}_i(t)) \tag{9}$$

and let N grow. As the number N of the particles of this *unique* system tends to infinity, a non-singular one-particle probability distribution (in μ space) must be constructed[5] Using Eq.(9), and assuming that the physical space is d-dimensional, this can be done introducing a cell size Δ in μ space, such that $N \gg \Delta^{-2d}$, i.e.

[5]This is needed for the Boltzmann entropy to exist, like a non-singular distribution in Γ space is required for the Gibbs entropy to exista

that there is a statistically relevant number of particles in each cell. Then, define the one-particle coarse grained distribution:

$$f_\Delta(\mathbf{q}^{(j)}, \mathbf{p}^{(k)}, t) = \frac{1}{N}\sum_{i=0}^{N} \Theta\left(1 - \frac{2|\mathbf{q}^{(j)} - \mathbf{q}_i(t)|}{\Delta}\right)\Theta\left(1 - \frac{2|\mathbf{p}^{(k)} - \mathbf{p}_i(t)|}{\Delta}\right) \quad (10)$$

where $\Theta(z)$ is the Heaviside step function and $\mathbf{q}^{(j)}$, $\mathbf{p}^{(k)}$ are the coordinates of the center of each cell C_{jk} having linear size Δ, and volume Δ^{2d}, in the appropriate units. The Boltzmann entropy is then defined by

$$S_B(t) = -k_{_B}\int f(\mathbf{q}, \mathbf{p}, t)\ln f(\mathbf{q}, \mathbf{p}, t)\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} \quad (11)$$

where f is the regular μ-space probability distribution, obtained in the $N \to \infty$, $\Delta \to 0$ limit of Eq.(10). The Boltzmann entropy, as defined in Eq.(11), is a natural candidate for the description of dilute systems, for which it represents the logarithm of the volume occupied by the macrostate in the Γ space:

$$S_B = k_{_B}\log \Delta\Gamma. \quad (12)$$

Moreover, for dilute systems under the hypothesis of molecular chaos the celebrated Boltzmann's H-theorem holds:

$$\frac{dS_B}{dt} \geq 0. \quad (13)$$

The validity of the molecular chaos hypothesis has been demonstrated for the class of dilute systems in the Grad limit, where $N \to \infty$ and the interaction range goes to zero in order to keep the total cross section constant [22, 24].

Some textbooks try to connect the two main approaches noticing that in dilute systems:

$$\rho(\mathbf{X}, t) \simeq \prod_{j=1}^{N} f(\mathbf{q}_j, \mathbf{p}_j, t) \quad (14)$$

which implies that $S_G \simeq NS_B$. This attempt, however, is only partially justified, as there are at least two important conceptual differences between these approaches:

- The Gibbs point of view is based on the ensemble, i.e. on an abstract collection of macroscopically identical systems, and does not depend on the number of particles of which each system is made. Differently, Boltzmann's approach does not require an ensemble of copies of the same system, but needs $N \gg 1$, in order to compute $f(\mathbf{q}, \mathbf{p}, t)$ for the single system.

- The Gibbs entropy deals with the Γ space, and necessitates a coarse graining procedure in order to avoid the consequences of the Liouville theorem, and to grow during an irreversible evolution. In the Boltzmann approach, the entropy can grow despite the Liouville theorem, and the graining of the μ-space is only introduced to deal with a smooth distribution.

In addition, the validity of (14) must be interpreted *cum grano salis*, otherwise, because of (13), one would erroneously infer that the Gibbs entropy (4) grows.

In the following, we will show that for long enough times, and non-vanishing interaction, the growth of S_B does not depend on the cell size, which is not the case for non-interacting systems.

3 The Boltzmann entropy of a chaotic system

3.1 The discrete time model

In order to discuss the points mentioned above in a concrete fashion, let us start with a system consisting of $N \gg 1$ non-interacting particles moving in a periodic array of fixed convex scatterers, with which they collide elastically.

The position of the scatterers should avoid the presence of collisionless trajectories, i.e. the horizon should be finite. It is well established that such a system, commonly known as the Lorentz gas[6] is chaotic and displays asymptotic diffusion. The Gibbs entropy of such a system obeys $S_G(t) = S_G(0)$, while the coarse-grained entropy increases linearly with t for $t > t_\lambda$ (before saturation). It is easy to see that $h_{KS} = Nh_1$, where h_1 is the Kolmogorov-Sinai entropy of a single particle, and $S_B = (S_G)/N$ = constant, because the particles are independent, and the probability distribution in phase space factorizes in N identical terms.

The situation is quite different in the case of interacting particles, such as the case of the generalization of the Lorentz gas given in Ref.[25]. There, the particles are not point-like, but have a finite size, and therefore they collide not only with the scatterers, but also among themselves.

Unfortunately, the study of such a system, for a sufficiently large number of particles, is very expensive from a computational point of view. However, a reasonable substitute for such a system, which shares its main features, can be given in terms of symplectic maps. For instance, one can consider a two-dimensional map, with one "coordinate" and one "momentum", in place of each particle of the generalized Lorentz gas, and one can introduce a form of interaction among these "particles". Thus we require that:

- in the absence of interactions among the "particles", the single-particle dynamics in the corresponding μ space be chaotic and volume preserving;
- in the presence of interactions among particles, the dynamics of the whole system, described by the vector $\mathbf{X} = (\mathbf{Q}, \mathbf{P})$, $\mathbf{Q} = (q_1 \dots q_n)$, $\mathbf{P} = (p_1 \dots p_n)$, be symplectic and volume preserving in the Γ space.

The resulting model will be numerically easier to handle, still having some important properties of the particle system. In particular, the dynamics of the interacting

[6] In Lorentz's original model, the moving particles were considered in thermal equilibrium with the scatterers, which is impossible to achieve without energy exchanges between scatterers and particles, as in the present model.

case will not be volume preserving in the μ space. To this aim, we introduce the symplectic map:

$$\begin{cases} q_i &= \partial G(\mathbf{Q}', \mathbf{P})/\partial p_i \quad \mod 1 \\ p_i' &= \partial G(\mathbf{Q}', \mathbf{P})/\partial q_i' \quad \mod 1 \end{cases} \tag{15}$$

whose generating function $G(\mathbf{Q}', \mathbf{P})$ is defined by:

$$G(\mathbf{Q}', \mathbf{P}) = \mathbf{Q}'\mathbf{P} - \frac{|\mathbf{P}|^2}{2} - \frac{k}{2\pi} \sum_{i=0}^{N} \sum_{j=0}^{N_S} \cos\left[2\pi(q_i' - Y_j)\right] - \\ - \frac{\epsilon}{4\pi} \sum_{i=0}^{N} \sum_{n=-M/2}^{M/2} \cos\left[2\pi(q_i' - q_{i+n}')\right] \tag{16}$$

with $q_i, p_i \in [0, 1]$. N_S is the number of fixed "obstacles" having positions Y_j, which play the role of the convex scatterers in the Lorentz gas, and N is the number of "particles". The parameters k and ϵ represent the interaction strength between particles and obstacles and among particles respectively. If $k = \epsilon = 0$ one has free particles. The functional form of the generating function is reminiscent of the standard map, which is a paragon of symplectic dynamics. The boundary conditions on the variables are periodic, and the form of the interactions does not present discontinuities at the boundaries. In order to make the numerical simulations faster, we assume that each particle interacts only with a limited number M of other particles.

Substituting Eq.(16) into (15), one finds:

$$\begin{cases} q_i' = & q_i + p_i \quad \mod 1 \\ p_i' = & p_i + k \sum_{j=0}^{N_S} \sin[2\pi\,(q_i' - Y_j)] + \epsilon \sum_{n=-\frac{M}{2}}^{\frac{M}{2}} \sin[2\pi\left(q_i' - q_{i+n}'\right)] \quad \mod 1 \end{cases} \tag{17}$$

Since the system is symplectic, the dynamics described by the points $(\mathbf{Q}, \mathbf{P})$ will preserve volumes in phase space.

3.2 Numerical results

In the following, we calculate the Boltzmann single-particle distribution for a given cell size (cf. Eq.(10)), as a function of time. Then, we study the growth of the corresponding Boltzmann entropy with time, defined by

$$S_B(t, \Delta) = -k_B \sum_{j,k} f_\Delta(q^{(j)}, p^{(k)}, t) \log f_\Delta(q^{(j)}, p^{(k)}, t) \tag{18}$$

by varying the interaction strength ϵ and the cell size Δ. Note that, in our numerical computations, where we set $k_B = 1$ for convenience, there are no *a priori* assumptions such as, for example, the hypothesis of molecular chaos. In other words, the quantity $f_\Delta(q, p, t)$ evolves according to the exact dynamics.

Let us comment on the use of the entropy defined in Eq.(18) for our dynamical system. As discussed in the Introduction, this expression is correct (in the sense that it measures the interesting volume of phase space) only in the case of dilute systems. For systems, where the potential energy is not a tiny fraction of the total, it has been proposed [21, 26] that a similar recipe may still be used, with the prescription to count only microstates corresponding to a fixed total energy E. Since we are considering the case of weakly interacting subsystems, the function $f(q, p, t)$ is able to properly describe the macrostates of the system

First of all, we choose the number of obstacles N_S and the parameter k (both related to the single-particle chaotic behavior) in such a way that a) the Lyapunov exponent of the single particle dynamics is not too large and b) there are no KAM tori, of the kind which constitute barriers for the transport. One possible choice, which realizes this requirement is $N_S = 10^3$ and $k = 0.017$. The obstacles positions are selected at random, with a uniform p.d.f. The result is that the Lyapunov exponent is $\lambda \approx 0.162$. An example of a trajectory in the 1-particle (q, p) space is shown in Fig.1.

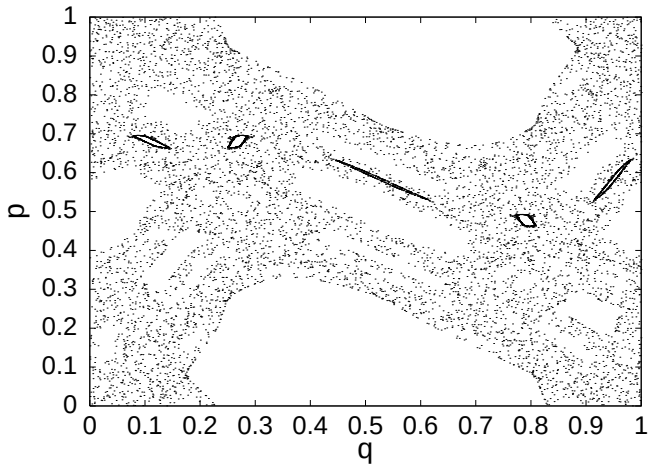

Figure 1: A trajectory generated by 10^4 map iterations in the phase space of a single particle, with $N_S = 10^3$, $k = 0.017$,$\epsilon = 0$.

For the number of particles, we chose $N = 10^7$, after checking that finite size effects are negligible for this N, and we let the simulations run for different values of ϵ. We checked that the results basically do not change when the number of particles is reduced by a factor 10. As initial non-equilibrium condition, we take a cloud of points distributed according to a Gaussian of r.m.s.d $\sigma = 0.01$, having the point $(q, p) = (1/4, 1/2)$ as a center (we checked that this point is far enough from the surviving regular islands, see Fig. 1). At each time, we compute the differences between the entropy and its initial value at several resolutions Δ :

$$\delta S(t, \Delta) = S(t, \Delta) - S(0, \Delta). \tag{19}$$

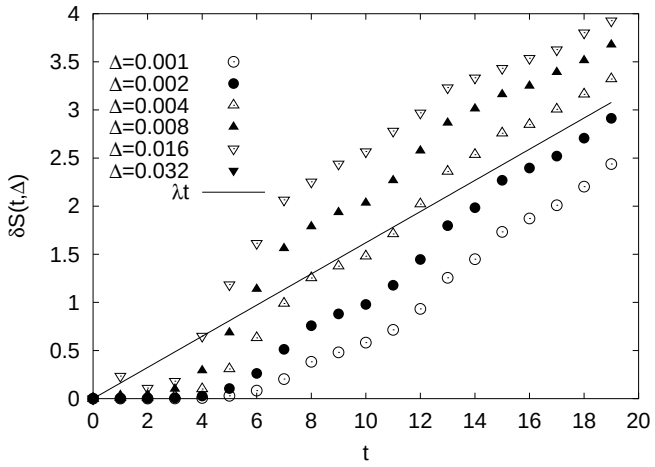

Figure 2: $\delta S(t,\Delta)$ with $\epsilon = 0$ (non-interacting particles) as a function of t for different values of Δ. The slope of the straight line equals Lyapunov exponent.

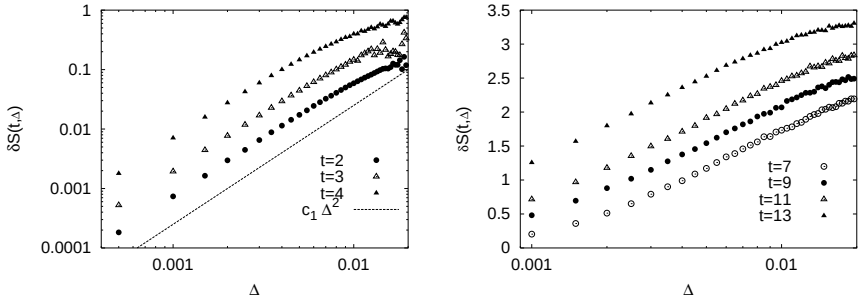

Figure 3: $\delta S_B(t,\Delta)$ with $\epsilon = 0$ (non-interacting particles) as a function of Δ, for small values of t (left) and large values of t (right). In the left panel, the dotted line shows the expected behavior $\delta S_B(t,\Delta) \propto \Delta^2$, while the logarithmic behavior is clearly visible in the right panel (notice the log-linear scale).

We begin with the study of the $\epsilon = 0$ case. The entropy growth shown in Fig.2 is only due to the discretization procedure, since the equation ruling the evolution of $f(q,p,t)$ obeys the Liouville theorem. This means that the "true" Boltzmann entropy for $\Delta \to 0$ is constant in time. As shown in Fig.2, the curves of the entropy differences as functions of time stay constant up to a time t_λ depending on Δ. After this transient, the slope of $\delta S(t,\Delta)$ is practically the same for all the curves and is approximately given by h_{KS} (see Eq.7). Looking at the curves of the entropy differences as a function of Δ (see Fig.3), it is possible to extrapolate the behavior for $\Delta \to 0$: far from the saturation (i.e. for small times) and for Δ not too large, these curves are well fitted by a power law:

$$\delta S_B(t,\Delta) \propto \Delta^2. \tag{20}$$

This result suggests that the relevant parameter for understanding the finite res-

olution behavior of the entropy differences is the cell area Δ^2; moreover, these differences go correctly to zero when $\Delta \to 0$. For t larger than t_λ, one observes

$$\delta S_B(t, \Delta) = a \log(\Delta) + b. \tag{21}$$

Of course, the behavior of Eq. (20) and (21) is consistent with Eq.(7), taking into account that the rate of entropy growth after t_λ is generally different from the Lyapunov exponent, leading to $a \neq 1$ [23].

We consider now the "interacting" case, i.e. $\epsilon > 0$. Figure 4 and 5 show the curves of $\delta S_B(t, \Delta)$ as a function of t and Δ. In this case, the entropy curves as a function of Δ do not extrapolate anymore to zero (see Fig. 5); these curves, for small (fixed) times, are well fitted by a polynomial like:

$$\delta S_B(t, \Delta) \approx c_0 + c_1 \Delta^2. \tag{22}$$

After a characteristic time depending on ϵ, $t_*(\epsilon, \Delta)$, the entropy shows just a weak (logarithmic) dependence on Δ and correctly extrapolates to a finite value when $\Delta \to 0$.

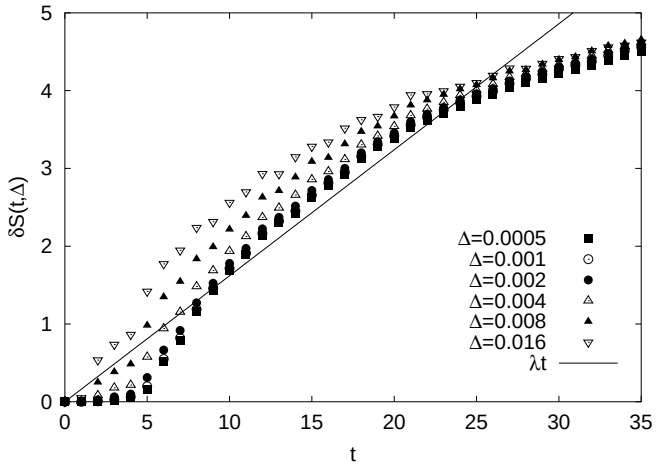

Figure 4: $\delta S_B(t, \Delta)$ with $\epsilon = 10^{-4}$ as a function of t for different values of Δ. The straight line slope equals the Lyapunov exponent.

Let us now summarize and comment the previous results:

a) for non-interacting systems ($\epsilon = 0$), the growth of $\delta S_B(t, \Delta)$ reflects the properties of the observation tools, i.e. $\delta S_B \simeq 0$ for $t \lesssim t_\lambda(\Delta)$ and $\delta S_B \simeq \lambda(t - t_\lambda(\Delta))$ for $t \gtrsim t_\lambda(\Delta)$, has a kind of "subjective" character. Since t_λ increases as Δ decreases, not only does the value of the entropy depend on the coarse graining, but the entropy growth depends (for "small" t) on the resolution scale, as noticed in [14].

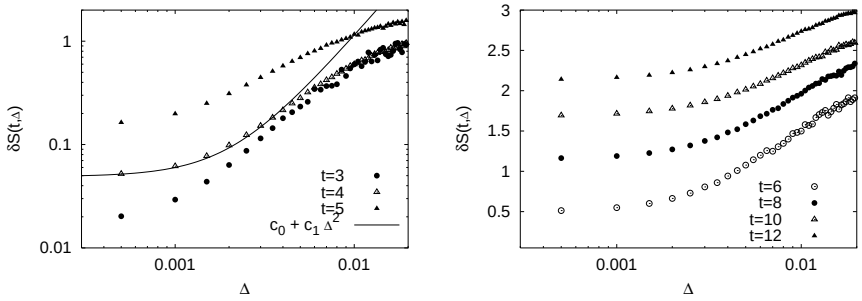

Figure 5: $\delta S_B(t,\Delta)$ with $\epsilon = 10^{-4}$ as a function of Δ for small values of t (left panel) and large values of t (right panel). In the left panel the line shows the expected behavior $c_0 + c_1\Delta^2$ while in the right panel $\delta S_B(t,\Delta)$ shows a weak dependence on Δ for $\Delta \to 0$.

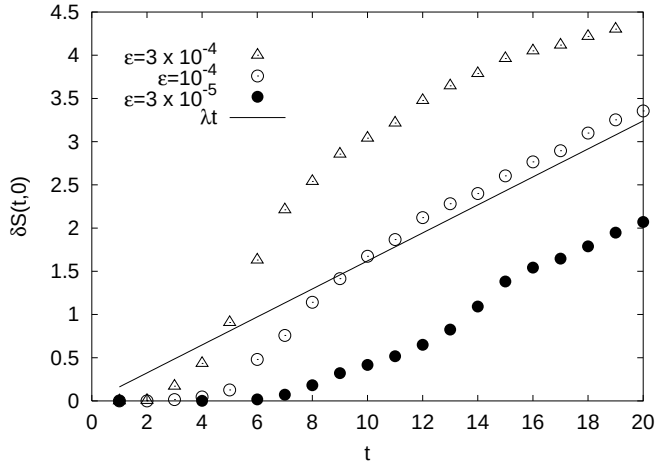

Figure 6: Extrapolation for $\Delta \to 0$ of the curves $\delta S_B(t,\Delta)$ as a function of t for various values of ϵ.

b) For weakly interacting systems, there is an effective cell size $\Delta_*(\epsilon,\lambda)$, such that if $\Delta < \Delta_*(\epsilon,\lambda)$ the value of $\delta S_B(t,\Delta)$ does not depend on Δ. Here, the entropy growth is an objective property, meaning that the limit for $\Delta \to 0$ of $\delta S_B(t,\Delta)$ exists, is finite, hence is an intrinsic property of the system (cf. Fig.5).

c) The role of chaos in the limit of vanishing coupling is relevant, i.e. the slope of $\delta S_B(t,\Delta)$, for t large enough, is given by the Lyapunov exponent, but the existence of an effective cell size $\Delta_*(\epsilon,\lambda)$ and the corresponding $t_*(\epsilon,\lambda)$ depends on the coupling strength ϵ, and on λ.

d) In the above procedure, i.e. in the evaluation of Eqs. (10) and (18), there are no assumptions like the hypothesis of molecular chaos or of system's dilution.

From a mathematical point of view, we can define $S_B(t, \Delta)$ in Eq.(18) in full generality. However, we consider only the weakly interacting limit of small ϵ for the physical reason that only in such a case does $f(q, p, t)$ afford an appropriate thermodynamic meaning.

e) For small values of ϵ, the time evolution of $f(q, p, t)$ is different from the case $\epsilon = 0$ only on very small graining scales; in other words, the coupling is necessary for the "genuine" growth of the entropy, but it does not have any dramatic effect on $f(q, p, t)$ at scales $\Delta \lesssim \Delta_*$. Indeed, as shown in Fig.7, the noninteracting and the weakly interacting cases do not appear to be so different, in terms of the single-particle phase space distribution.

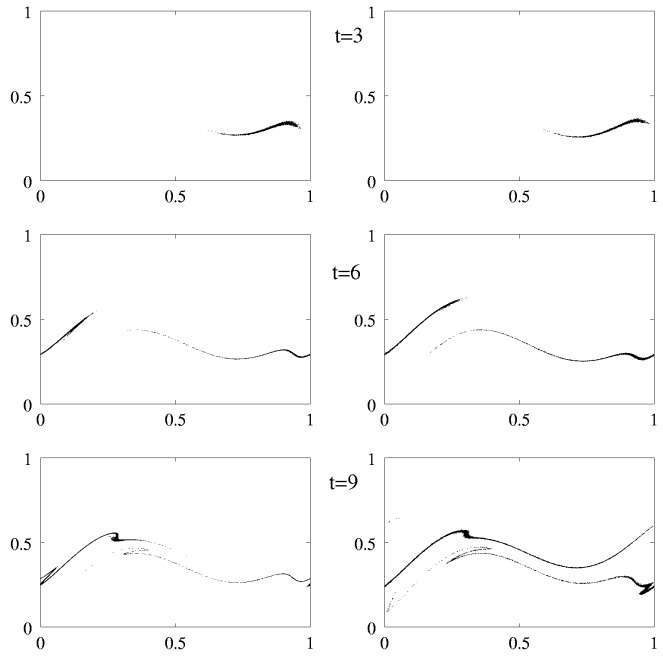

Figure 7: Snapshots of the evolution of the system in the single-particle projection of the phase space in the non-interacting case (left), and in the interacting case with $\epsilon = 10^{-4}$ (right) and $M = 100$, at increasing times from top to bottom, as indicated in the figure.

4 Interpretation of the results

The results of the previous section suggest the following interpretation: since the number of particles is large, one can expect that the effect of the interaction on each particle may be reasonably described by some kind of thermal bath. The single

particle dynamics can then be mimicked by chaotic dynamics (corresponding to the symplectic map of Eq.(17) with $\epsilon = 0$) coupled to a noise term whose strength is $O(\epsilon)$:

$$\begin{cases} q_i(t+1) &= q_i(t) + p_i(t) & \mod 1 \\ p_i(t+1) &= p_i(t) + k\sum_j \sin\left[2\pi(q_i(t+1) - Y_j)\right] + \sqrt{2D}\eta_i(t) & \mod 1 \end{cases} \tag{23}$$

where $\eta_i(t)$'s are i.i.d. Gaussian variables with zero mean and unitary variance, i.e.

$$\langle \eta_i(t) \rangle = 0, \quad \langle \eta_i(t)\eta_j(t') \rangle = \delta_{t,t'}\delta_{i,j}. \tag{24}$$

With this approximation, one basically assumes that $f(q, p, t)$ evolves according to a discrete time Fokker-Planck equation. Supposing that each particle gives an uncorrelated contribution to the noise term, one can roughly estimate the diffusion coefficient D as $M\epsilon^2/4$. This heuristic estimate is well supported by numerical simulations of (17): the quantity $\delta S_B(t, \Delta)$ practically does not change at varying M and ϵ, keeping $M\epsilon^2$ constant.

In this framework, one can introduce a characteristic time t_c, defined as the time in which the scale of the noise induced diffusion reaches the smallest scale originated by the deterministic chaotic dynamics [27]. This definition of t_c would correspond to $t_*(\epsilon, \lambda)$ introduced above. Consequently, noting that the typical lengths due to noise and to chaos behave as $\sqrt{M\epsilon^2 t/2}$ and $\sigma \exp(-\lambda t)$, respectively, the time t_c may be estimated as the solution of the following transcendent equation:

$$\epsilon\sqrt{Mt_c/2} = \sigma \exp(-\lambda t_c) \tag{25}$$

which holds on the spatial scales already reached by the diffusion process:

$$\epsilon\sqrt{Mt/2} > \Delta \ , \tag{26}$$

beyond which the value of the entropy still depends on the size of Δ (i.e. the curves $S_B(\Delta)$ display the behavior $S_B(t, \Delta) \sim \Delta^2$). For example, in the case with $\epsilon = 10^{-4}$, $\sigma = 0.01$, $M = 100$ and $\lambda = 0.162$, one obtains $t_c \simeq 9$, and, in agreement with our interpretation, for $t > 9$, all the curves in Fig.6 present the same slope compatible with the Lyapunov exponent λ.

As a numerical check of the consistency of this approach, we studied system (23). The results with a given D should be compared with those of the deterministic system of Eq.(17) with

$$\epsilon = \epsilon_{eq} \equiv 2\sqrt{\frac{D}{M}}. \tag{27}$$

The results, shown in Fig.8 and 9, are qualitatively similar to the deterministic interacting case (17), confirming the validity of our approach.

A similar reasoning leads to the decoherence mechanism proposed by Zurek and Paz [28] for the semiclassical limit of quantum mechanics. We note that rather subtle conceptual points are present in the decoherence process for the semiclassical

limit. This is so because two theories are involved (classical and quantum mechanics) with very different ontological status (deterministic and non-deterministic, respectively). In our problem one has just a technical aspect: roughly speaking, one mimics the first equation of the BBGKY hierarchy of a diluted system, consisting of weakly interacting chaotic particles, with a suitable Fokker-Planck equation.

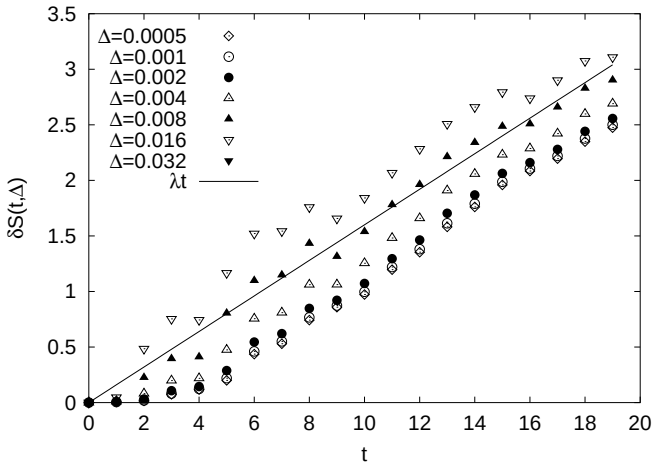

Figure 8: Numerical simulation of $N = 10^7$ independent particles evolving according to (23) with $\epsilon_{eq} = 10^{-4}$. Notice the similar qualitative behavior observed in Fig.(4).

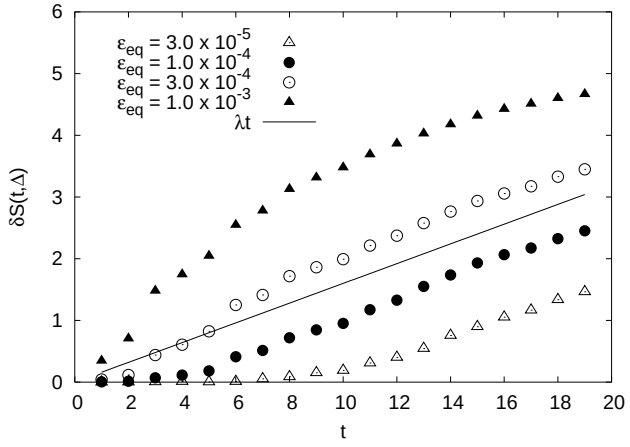

Figure 9: Extrapolation for $\Delta \to 0$ of the curves $\delta S_B(t, \Delta)$ as a function of t for various values of ϵ_{eq}. Notice that the extrapolated curves are qualitatively similar to the interacting case (cf. Fig. 6).

5 Conclusions and perspectives

We have studied a system made of weakly coupled chaotic subsystems, which can be considered as a model of weakly interacting particles in an environment with convex obstacles. In the non interacting limit the behavior of the Boltzmann entropy depends strongly on the coarse-graining resolution (*i.e.* the cell size Δ) and therefore it cannot be considered an intrinsic property of the system. By contrast, in the weakly interacting case the behavior of the Boltzmann entropy becomes independent of the observation scale, assuming an objective character: for Δ small enough, *i.e.* smaller than $\Delta_*(\epsilon, \lambda)$, one observes a well defined shape of $\delta S_B(t)$ *vs* t. A remarkable fact is that $\delta S_B(t)$, for $t \gtrsim t_*(\epsilon, \lambda)$, increases roughly linearly, with a slope given by the Kolmogorov-Sinai entropy of the single (non interacting) chaotic system. Summarizing, the interaction is necessary in order to have an effective cell size Δ_*, thus changing the time behavior of the Boltzmann entropy from "subjective" to "objective", while other numerical aspects, like the slope of $\delta S_B(t)$for $t \gtrsim t_*$, are basically determined by the degree of chaos in the single subsystems. In addition, the effect of the weak coupling among the chaotic subsystems can be successfully modeled with a noisy term, and this allows us to estimate the value of $t_*(\epsilon, \lambda)$.

Let us now comment on the relevance of these results for the case of noninteracting particles, in a host environment made of very heavy particles. If the "obstacles" were not infinitely massive, they would exchange energy with the independent particles, like the case of photons in a black body cavity. The photons do not interact with each other, but interact with the walls, reach a thermal equilibrium with them, and acquire a temperature for themselves. A similar behavior has been obtained in the Lorentz-like model of Ref.[29]. In our framework, this would amount to set the interaction ϵ to zero, and to switch on an interaction between particles and obstacles which now are allowed to move. Denoting with Y_J and W_J the coordinate and the momentum of the J-th obstacle, one can introduce a symplectic dynamics, which generalizes (15) introducing a suitable interaction among the "light" particles and the heavy obstacles. Of course now the Γ space is given by $(\mathbf{Q}, \mathbf{Y}; \mathbf{P}, \mathbf{W})$. Then, the "light" particles would be indirectly coupled with each other, as in [29]: indeed, the heavy particles will play the role of interaction carrier particles and essentially we would fall back in the case considered in this paper. Clearly, an interaction carried by heavy particles will be very weak and will involve very small scales, which are difficult to observe in numerical simulations; nevertheless, there are no reasons to expect any conceptual difference from the scenario described in the present paper, which is consistent with the results of Ref.[29].

Of course, our results do not rule out noninteracting particle systems from the class of physically relevant models. In fact, they can be quite useful in describing highly rarefied gases, such as those of high vacuum pumps, or in the upper layers of the atmosphere. Recently, they have also proven to be useful in the description of transport in microporous membranes [17], which are of a strong technological

interest. Therefore, credit must be given to those who have analyzed, and popularized these models, in the framework of nonequilibrium statistical mechanics (cf. [12, 13] and references therein). Similarly, we do not exclude that some version of the coarse-grained Gibbs entropies may serve as useful characterizations of the state of certain systems. Our results indicate that such systems, and such definitions of entropy, are not appropriate to understand, from a theoretical point of view, what happens in thermodynamic systems where the macroscopic evolutions toward equilibrium involve all the relevant microscopic degrees of freedom.

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